Table S1. (Deposited material): Overview of the known determinations of $KRES_2$, $RbRES_2$ and $M^+Sc^{3+}S_2$ compounds. (Red-typed parts indicate problems.)

$KLaS_2$	44942	01-089-4261	Ballestracci (1965)	$R\bar{3}m$	4.464	21.89(5)	3	Cell parameters from powder diffraction; Wrong parameter *b*, probably misprint; probably should be 4.264 (see also Ballestracci & Bertaut (1965); in ICSD and PDF4 is given *a*=*b*=4.464 Å, *c*=21.89499 Å, *z*(S)=0.256; the structure taken from ICSD. The structure is not given in the referenced article.
$KLaS_2$			Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.264	21.89(5)	3	
$KLaS_2$			Fábry *et al.* (2014*a*)	$R\bar{3}m$	4.2651(4)	21.929(3)	3	*z*(S)=0.23718(11)/ $K_{0.971(8)}La_{1.020(5)}S_{2.00(1)}$ 3 points by electron microprobe
$KCeS_2$	351	00-030-0922/ 04-008-8072	Plug & Verschoor (1976)	$R\bar{3}m$	4.228(4)	21.80(1)	3	*z*(S)= 0.26346(4), single crystal determination; in ICSD the lattice parameter *c*=21.80(2) Å. The lattice parameters in the referenced files are given as *a*=*b*=4.228 and *c*=21.8 Å
$KCeS_2$	621439		Ballestracci (1965)/ Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.223	21.80	3	Cell parameters from powder diffraction; the structure is given in ICSD but not in the original article by Ballestracci (1965): "Coordinates estimated by the editor in analogy to isotypic compounds."

$KPrS_2$	44943	01-089-4262	Ballestracci (1965)/ Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.185	21.75	3	Cell parameters from powder diffraction; z(S)=0.265; the structure was taken from ICSD, but it is not given in the referenced article by Ballestracci (1965).
$KPrS_2$			Fábry *et al.* (2014*a*)	$R\bar{3}m$	4.1925(3)	21.8920(14)	3	z(S)=0.23618(7); $K_{0.941(1)}$ $Pr_{1.004(4)}$ $S_{2.000(5)}$, 3 points by electron microprobe/16kV
$KNdS_2$			Verheijen *et al.* (1975)	$R\bar{3}m$				*z*(S)=0.2647(5); neutron diffraction; lattice parameters not given.
$KNdS_2$	641272		Ballestracci (1965)	$R\bar{3}m$	4.160(5)	21.83		Cell parameters from powder diffraction; In ICSD the lattice parameters given as a=4.1605, c=21.83; *z*(S)=0.265 estimated by an editor of ICSD.
$KNdS_2$			Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.161	21.83		Cell parameters from powder diffraction
$KNdS_2$			This study	$R\bar{3}m$	4.1626(3)	21.8996(19)		z(S)=0.23595(4), X-ray single crystal determination.
$KPmS_2$								
$KSmS_2$	44944	01-089-4263	Ballestracci (1965)/ Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.107	21.76	3	Cell parameters from powder diffraction; in ICSD as well as in PDF-4 wrong unit cell parameters (4.107 and 21.75999); *z*(S)=0.268; the structure is given in ICSD but not in the original article by Ballestracci (1965).
$KSmS_2$			This study	$R\bar{3}m$	4.1174(6)	21.888(3)	3	*z*(S)=0.23520(16)

$KEuS_2$	631365		Ballestracci (1965)	$R\bar{3}m$	4.093	21.85(5)	3	*z*(S)=0.268, the structure is given in ICSD but not in the original article. "Coordinates estimated by the editor in analogy to isotypic compounds." In ICSD the *c*-parameter is given as 21.855 Å.
$KEuS_2$			Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.093	21.85(5)	3	
$KEuS_2$			Fábry *et al.* (2014a)		4.0981(3)	21.8212(15)		Single X-ray determination; *z*(S)= 0.23536(4)/ $K_{0.935(46)}Eu_{0.955(98)}S_{2.00(6)}$ 3 points by electron microprobe/16kV
$KGdS_2$	44945	01-089-4264	Ballestracci (1965)	$R\bar{3}m$	4.075	21.89	3	Cell parameters from powder diffraction; *z*(S)=0.267; the structure is given in ICSD but not in the original article by Ballestracci (1965).
$KGdS_2$			Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.075	22.89	3	An evident misprint regarding the axis *c*; it should be 21.89 Å
$KGdS_2$			Fábry *et al.* (2014*a*)-unpublished	$R\bar{3}m$	4.0619(7)	21.894(4)	3	*z*(S)= 0.23499(11)
$KGdS_2$			Fábry *et al.* (2014*a*)-unpublished	$R\bar{3}m$	4.0761(7)	21.894(3)	3	*z*(S)= 0.23508(10)
$KGdS_2$			Fábry *et al.* (2014*a*)		4.0715(7)	21.901(4)	3	z(S)= 0.23501(17)/ $K_{0.9296(36)}Gd_{0.98(3)}S_{2.00(3)}$ 4 points by electron microprobe/20kV
$KTbS_2$	641329		Ballestracci (1965)	$R\bar{3}m$	4.051	21.87	3	z(S)=0.269; the structure is given in ICSD but not in the original article by Ballestracci (1965). ("Coordinates estimated by the editor in analogy to isotypic

								compounds.").
$KTbS_2$			Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.051	21.87	3	
$KTbS_2$			This study	$R\bar{3}m$	4.0523(7)	21.885(3)	3	z(S)=0.23463(9)
$KDyS_2$	44946	01-089-4265	Ballestracci (1965)/	$R\bar{3}m$	4.030	21.83	3	Cell parameters from powder diffraction; in ICSD and PDF-4 there are given the unit cell parameters 4.03 and 21.82999 Å; *z*(S)=0.269; the structure is given in ICSD but not in the referenced article by Ballestracci (1965).
$KDyS_2$	44946		Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.030	21.83	3	Cell parameters from powder diffraction; in ICSD and PDF-4 there are given the unit cell parameters 4.03 and 21.82999 Å; *z*(S)=0.269; the structure is given in ICSD but not in the referenced article by Ballestracci (1965).
$KDyS_2$			This study	$R\bar{3}m$	4.0315(11)	21.890(5)	3	z(S)=0.2345(3)
$KHoS_2$	44947	01-089-4266	Ballestracci (1965)	$R\bar{3}m$	4.009(5)	21.80	3	Cell parameters from powder diffraction; in ICSD as well as in PDF-4 wrong unit cell parameters 4.0095 and 21.79999, *z*(S)=0.27; the structure given in ICSD is not given in the referenced article by Ballestracci (1965).
$KHoS_2$	639366		Verheijen *et al.* (1975)	$R\bar{3}m$	4.010	21.80	3	Lattice parameters taken from Ballestracci & Bertaut (1965).

								z(S)=0.27 though the structure given in ICSD is not given in the referenced article by Verheijen *et al*. (1975). ("Coordinates estimated by the editor in analogy to isotypic compounds.").
$KHoS_2$			Ballestracci & Bertaut (1965)	$R\bar{3}m$	4.010	21.80	3	Taken from Ballestracci & Bertaut (1965). Colloques internationaux du C.N.R.S. Orsay 28 sept.-1.oct. 1965, 41-49.
$KHoS_2$			This study	$R\bar{3}m$	4.0098(4)	21.878(2)		*z*(S)=0.23430(11)
$KErS_2$	44948	01-074-5813/ 01-089-4267	Ballestracci (1965)	$R\bar{3}m$	3.993	21.77	3	Cell parameters from powder diffraction; in ICSD given wrong unit cell parameters: *c*=21.7699 Å. In ICSD is given *z*(S)=0.2705 but it is not given in the referenced article by Ballestracci (1965).
$KErS_2$	108429	01-074-5813/ 01-089-4267	Ballestracci (1965)/	$R\bar{3}m$	3.993	21.77	3	Cell parameters from powder diffraction; in ICSDthere is given *z*(S)=0.265 but it is not given in the referenced article by Ballestracci (1965).
$KErS_2$			Ballestracci & Bertaut (1965)	$R\bar{3}m$	3.993	21.77	3	Cell parameters from powder diffraction.
$KErS_2$			This study	$R\bar{3}m$	3.9935(4)	21.866(2)		*z*(S)=0.23407(17)
$KTmS_2$		04-001-8391	Tromme (1971)		3.977(4)	21.84(2)		In PDF-4 is given *z*(S)=0.231 but this value is not given in the

								referenced article.
$KTmS_2$			This study	$R\bar{3}m$	3.9761(5)	21.841(3)	3	*z*(S)=0.23376(11)
$KYbS_2$	44949	01-089-4268	Ballestracci (1965)	$R\bar{3}m$	3.964	21.82	3	Cell parameters from powder diffraction; in ICSD as well as in PDF-4 wrong unit cell parameters 3.964 and 21.81999 Å; in ICSD is given *z*(S)=0.271 but it is not given in the referenced article by Ballestracci (1965).
$KYbS_2$		01-089-4268	Ballestracci & Bertaut (1965)	$R\bar{3}m$	3.964	21.82	3	Cell parameters from powder diffraction.
$KYbS_2$			This study	$R\bar{3}m$	3.9615(8)	21.810(3)	3	z(S)=0.23346(19)
$KLuS_2$			Fábry *et al.* (2014*a*)	$R\bar{3}m$	3.9490(4)	21.871(3)	3	z(S)=0.23369(15)/ $K_{0.992(8)}Lu_{1.096(12)}Gd_{0.03(2)}S_{2.00(3)}$ / 4 points by electron microprobe/20kV
$KLuS_2$		04-001-8390	Tromme (1971)	$R\bar{3}m$	3.947(2)	21.79(2)	3	In PDF-4 there is given *z*(S)=0.231 but this value is not given in the referenced article. In PDF-4 the lattice parameters are given without the standard uncertainties.
KYS_2			Fábry *et al.* (2014*a*)	$R\bar{3}m$	4.0216(5)	21.884(4)	3	z(S)=0.23444(8)
KYS_2			Ballestracci (1965)	*R-3m*	4.022(5)	21.85(5)	3	
KYS_2			Ballestracci & Bertaut (1965)	*R-3m*	4.023	21.85(5)	3	
$KScS_2$		00-051-1228		$R\bar{3}m$	3.8139(2)	21.726(2)	3	
$KScS_2$			This study	$R\bar{3}m$	3.8106(3)	21.719(2)	3	z(S)=0.23113(6)

$RbLaS_2$	81394	04-011-4782	Bronger *et al.* (1996)	$R\bar{3}m$	4.296(1)	22.930(6)	3	Lattice parameters determined from a single crystal; *z*(S)=0.2337(1); In ICSD the lattice parameter *c*=22.9300(60) Å.
$RbLaS_2$			Bronger *et al.* (1973)	$R\bar{3}m$	4.292	22.89	3	Powder, Guinier cam.era
$RbLaS_2$	185320		Havlák *et al.* (2011)		4.28	22.9	3	In ICSD 185320 is given a=4.280 and c=22.95 Å. (Havlák *et al.* (2011) make reference to PDF #86-0693, *a* = 4.30; *c* = 22.95 Å.)
$RbCeS_2$	81395	04-011-4769	Bronger *et al.* (1996)	$R\bar{3}m$	4.249(3)	22.851(22)	3	Lattice parameters determined from a single crystal; *z*(S)=0.2334(3).
$RbCeS_2$	73546	01-073-9727	Bronger *et al.* (1993)	$R\bar{3}m$	4.249(5)	22.843(5)	3	Powder diffraction; single crystal determination : *z*(S)=0.2335(2).
$RbCeS_2$			Bronger *et al.* (1973)	$R\bar{3}m$	4.246	22.80	3	Powder, Guinier camera
$RbPrS_2$	81396	04-011-4770	Bronger *et al.* (1996)	$R\bar{3}m$	4.221(2)	22.897(9)	3	Lattice parameters determined from a single crystal; *z*(S)=0.2329(2); In ICSD the lattice parameter *c*=22.8970(90) Å.
$RbPrS_2$			Bronger *et al.* (1973)	$R\bar{3}m$	4.222	22.87	3	Powder, Guinier camera
$RbNdS_2$	81397	04-011-4771	Bronger *et al.* (1996)	$R\bar{3}m$	4.194(2)	22.894(12)	3	Lattice parameters determined from a single crystal; *z*(S)= 0.2327(1).
$RbNdS_2$			Bronger *et al.* (1973)	$R\bar{3}m$	4.189	22.89	3	Powder, Guinier camera
$RbPmS_2$								
$RbSmS_2$	81398	04-011-4772	Bronger *et al.* (1996))	$R\bar{3}m$	4.143(2)	22.880(9)	3	Lattice parameters determined from a single crystal; *z*(S)=0.2321(1); In ICSD, the lattice

								parameter *c*=22.880(9) Å.
$RbSmS_2$			Bronger *et al.* (1973)	$R\bar{3}m$	4.141	22.861	3	Powder, Guinier camera
$RbEuS_2$	81399	04-011-4773	Bronger *et al.* (1996)	$R\bar{3}m$	4.126(2)	22.890(12)	3	Lattice parameters determined from a single crystal; *z*(S)= 0.2319(1).
$RbEuS_2$			Bronger *et al.* (1973)	$R\bar{3}m$	4.119	22.84	3	Powder, Guinier camera
$RbGdS_2$	81400	04-011-4774	Bronger *et al.* (1996)	$R\bar{3}m$	4.110(1)	22.900(7)	3	Lattice parameters determined from a single crystal; *z*(S)= 0.2320(1); In ICSD, the lattice parameter *c*=22.8800(90) Å.
$RbGdS_2$			Bronger *et al.* (1973)	$R\bar{3}m$	4.098	22.88	3	Powder, Guinier camera
$RbTbS_2$	81401	04-011-4775	Bronger *et al.* (1996)	$R\bar{3}m$	4.080(1)	22.874(8)	3	Lattice parameters determined from a single crystal; *z*(S)= 0.2315(1) Bronger, W., Eyck, J., Kruse, K., Schmitz, D. Eur. J. Solid State Inorg. Chem. 33, 213,226 (1996); In ICSD, the lattice parameter *c*=22.8740(80) Å.
$RbTbS_2$		00-048-1725		$R\bar{3}m$	4.079(2)	22.870(4)	3	PDF-4 refers to the article by Bronger *et al.* (1996) – see above - but there are no such data..
$RbTbS_2$			Bronger *et al.* (1973)	$R\bar{3}m$	4.070	22.80	3	Powder; Guinier camera
$RbDyS_2$	81402	04-011-4776	Bronger *et al.* (1996)	$R\bar{3}m$	4.060(2)	22.885(18)	3	Lattice parameters determined from a single crystal; *z*(S)= 0.2312(1).
$RbDyS_2$			Bronger *et al.* (1993)	$R\bar{3}m$	4.052(7)	22.826(5)	3	
$RbDyS_2$		00-052-0883		$R\bar{3}m$	4.0531(2)	22.841(2)	3	
$RbHoS_2$	81403	04-011-4777	Bronger *et al.* (1996)	$R\bar{3}m$	4.037(3)	22.844(18)	3	Lattice parameters determined from a single crystal; *z*(S)= 0.2309(2).
$RbHoS_2$			Bronger *et al.* (1993)	$R\bar{3}m$	4.023(1)	22.753(7)	3	
$RbErS_2$	81404	04-011-4778	Bronger *et al.* (1996)	$R\bar{3}m$	4.026(3)	22.802(20)	3	Lattice parameters determined from a single

								crystal; *z*(S)= 0.2311(4).
$RbErS_2$			Bronger *et al.* (1993)	$R\bar{3}m$	4.017(1)	22.774(9)	3	
$RbTmS_2$	81405	04-011-4779	Bronger *et al.* (1996)	$R\bar{3}m$	4.020(1)	22.838(6)	3	Lattice parameters determined from a single crystal; *z*(S)= 0.2305(2).
$RbTmS_2$			Bronger *et al.* (1993)	$R\bar{3}m$	4.006(8)	22.847(7)	3	
$RbYbS_2$	81406	04-011-4780	Bronger *et al.* (1996)	$R\bar{3}m$	3.991(1)	22.717(7)	3	Lattice parameters determined from a single crystal; *z*(S)= 0.2308(1).
$RbYbS_2$			Bronger *et al.* (1993)	$R\bar{3}m$	3.985(1)	22.801(7)	3	
$RbLuS_2$	81407	04-011-4781	Bronger *et al.* (1996)	$R\bar{3}m$	3.991(1)	22.838(7)	3	Lattice parameters determined from a single crystal; *z*(S)= 0.2303(2).
$RbLuS_2$			Bronger *et al.* (1993)	$R\bar{3}m$	3.973(1)	22.818(5)	3	
$RbYS_2$			Fábry *et al.* (2014*a*)	$R\bar{3}m$	4.0444(3)	22.8267(16)	3	Single crystal determination; *z*(S)= 0.23090(15)/ $Rb_{0.875(36)}Y_{0.923(43)}S_{2.000(35)}$ / 4 points by electron microprobe/16kV.
$RbScS_2$			This study	$R\bar{3}m$	3.8299(6)	22.656(3)	3	z(S)=0.22811(10)

Compound	**ICSD**	**PDF-5**	**Reference**	**Space Group**	**a [Å]**	**c [Å]**	**Z**	**Note**
LiScS2	642305	00-041-0785	van Dijk & Plug (1980)	$R\bar{3}m$	3.687(1)	18.318(2)	3	*z*(S)=0.245 is given in ICSD but it is missing in the referenced article by van Dijk & Plug (1980). Coordinates were estimated by the editor in analogy to the isotypic compounds. In PDF5, *z*(S)=0.231. In

								the referenced article by van Dijk & Plug (1980), only powder diffraction experiment is mentioned in difference to ICSD.
NaScS2	644971	00-041-0786/ 04-004-0009	van Dijk & Plug (1980)	$R\bar{3}m$	3.751(1)	19.744(3)	3	*z*(S)=0.24 is given in ICSD but it is missing in the referenced article by van Dijk & Plug (1980). Coordinates were estimated by the editor. *z*(S)=0.231 in both hits of PDF5. In the referenced article by van Dijk & Plug (1980), only powder diffraction is mentioned in difference to ICSD.
KScS2		00-051-1228		$R\bar{3}m$	3.8139(2)	21.726(2)	3	
KScS2			This study	$R\bar{3}m$	3.8106(3)	21.719(2)	3	*z*(S)=0.23106(6)
$RbScS_2$			This study	$R\bar{3}m$	3.8299(6)	22.656(3)	3	z(S)=0.22811(10)
TlScS2	418474		Teske *et al*. (2007)	*P63/mmc*	3.761(3)	14.942(4)	2	Structure determined

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